

A Symplectic Method to Generate Multivariate Normal Distributions

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The AMAS group at the Paul Scherrer Institute developed an object oriented library for high performance simulation of high intensity ion beam transport with space charge^{1,2}. Such particle-in-cell (PIC) simulations require a method to generate multivariate particle distributions as starting conditions.

In a preceding publications it has been shown that the generators of symplectic transformations in two dimensions are a subset of the real Dirac matrices (RDMs) and that few symplectic transformations are required to transform a quadratic Hamiltonian into diagonal form^{3,4}.

Here we argue that the use of RDMs is well suited for the generation of multivariate normal distributions with arbitrary covariances. A direct and simple argument supporting this claim is that this is the “natural” way how such distributions are formed. The transport of charged particle beams may serve as an example: An uncorrelated gaussian distribution of particles starting at some initial position of the accelerator is subject to linear deformations when passing through various beamline elements. These deformations can be described by symplectic transformations.

Hence, if it is possible to derive the symplectic transformations that bring up these covariances, it is also possible to produce arbitrary multivariate normal distributions without Cholesky decomposition. The method allows the use of arbitrary uncoupled distributions. The functional form of the coupled multivariate distributions however depends in the general case on the type of the used random number generator. Only gaussian generators always yield gaussian multivariate distributions.

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I. INTRODUCTION

In Ref.⁴ the author presented a so-called “decoupling” method that is based on the systematic use the real Dirac matrices (RDMs) in coupled linear optics. The RDMs are constructed from four pairwise anti-commuting basic matrices with the “metric tensor” $g_{\mu\nu} = \text{Diag}(-1, 1, 1, 1)$, formally written as:

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2 g_{\mu\nu}. \quad (1)$$

The remaining 12 RDMs are constructed as products of the basic matrices as described in the appendix.

The use of the RDMs enables to derive a straightforward method to transform transport matrices, force matrices (“symplices”) and σ -matrices in such a way that the transformed variables are independent, i.e. decoupled.

The reverse is required to generate multivariate normal distributions: A transformation that transforms linear independent distributions of variables in such a way that a given covariance matrix is generated. The idea therefore is the following: Generate a set of independent normally distributed variables with given variances and apply the inverse of the decoupling transformation derived from the desired covariance matrix. This will couple the “independent” variables in exactly the desired way. The presented scheme assumes an even number of

variables since it is based on canonical pairs, i.e. position q_i and momentum p_i - but it is always possible to ignore one of those variables.

Since the method is based on pairs of canonical variables, the decoupling scheme always treats two pairs of variables at a time, resulting in the use of 4×4 -matrices. If more than four random variables are required, the decoupling can be used iteratively in analogy to the Jacobi diagonalization scheme for symmetric matrices⁴.

II. COUPLED LINEAR OPTICS

In this section we give a brief summary of the major concept. Given the following Hamiltonian function

$$H = \frac{1}{2} \psi^T \mathbf{A} \psi, \quad (2)$$

where \mathbf{A} is a symmetric matrix and ψ is a state-vector or “spinor” of the form $\psi = (q_1, p_1, q_2, p_2)^T$. The state vector hence contains two pairs of canonical variables. The equations of motion (EQOM) then have the familiar form

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i}, \end{aligned} \quad (3)$$

or in vector notation:

$$\begin{aligned} \dot{\psi} &= \gamma_0 \nabla_\psi H \\ &= \mathbf{F} \psi \end{aligned} \quad (4)$$

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where the *force matrix* \mathbf{F} is given as $\mathbf{F} = \gamma_0 \mathbf{A}$. The matrix γ_0 is the symplectic unit matrix (sometimes labeled \mathcal{J} or \mathcal{S}) and is identified with the real Dirac matrix γ_0 (see appendix). We define the symmetric matrix of second moments σ containing the variances as diagonal and the covariances as off-diagonal elements. The matrix \mathbf{S} is simply defined as the product of σ with γ_0 :

$$\mathbf{S} = \sigma \gamma_0. \quad (5)$$

Both matrices, \mathbf{F} and \mathbf{S} , fulfill the following equation (using $\gamma_0^T = -\gamma_0$ and $\gamma_0^2 = -\mathbf{1}$):

$$\mathbf{F}^T = \gamma_0 \mathbf{F} \gamma_0. \quad (6)$$

Matrices that obey Eq. 6 have been named *symplices*, but they are also called “infinitesimally symplectic” or “Hamiltonian” matrices⁵. Symplices allow superposition, i.e. any sum of simplices is a simplex, but only the product of anti-commuting simplices is a simplex³.

Any real-valued 4×4 -matrix \mathbf{M} can be written as a linear combination of real Dirac matrices (RDM):

$$\mathbf{M} = \sum_{k=0}^{15} m_k \gamma_k. \quad (7)$$

The RDM-coefficients m_k can be computed from the matrix \mathbf{M} by:

$$m_k = \frac{\text{Tr}(\gamma_k^2)}{32} \text{Tr}(\mathbf{M} \gamma_k + \gamma_k \mathbf{M}), \quad (8)$$

where $\text{Tr}(\mathbf{X})$ is the trace of \mathbf{X} .

Hence the RDMs form a complete system of all real 4×4 -matrices, but only ten RDMs fulfill Eq. 6 and are therefore simplices: The basic matrices $\gamma_0, \dots, \gamma_3$ and the six “bi-vectors”, i.e. the six possible products of two basic matrices. The simplices are the generators of symplectic transformations, i.e. the generators of the symplectic group.

As well-known, the Jacobi matrix of a canonical transformation is symplectic, i.e. it fulfills the following equation^{5,6}:

$$\mathbf{M} \gamma_0 \mathbf{M}^T = \gamma_0. \quad (9)$$

The EQOM have the general solution

$$\psi(t) = \mathbf{M}(t, t_0) \psi(t_0), \quad (10)$$

where \mathbf{M} is a symplectic *transfer matrix* that is in case of constant forces given by

$$\mathbf{M}(t, t_0) = \exp(\mathbf{F}(t - t_0)). \quad (11)$$

Given now an (initial) set of N normally distributed uncorrelated random variables ψ_i , then the σ -matrix of these variables is given by

$$\sigma = \frac{1}{N} \sum_{i=0}^{N-1} \psi_i \psi_i^T \equiv \langle \psi \psi^T \rangle, \quad (12)$$

where the superscript “T” indicates the transpose, then the distribution at time t is given by:

$$\sigma_t = \frac{1}{N} \sum_{i=0}^{N-1} \mathbf{M} \psi_i \psi_i^T \mathbf{M}^T = \mathbf{M} \sigma_0 \mathbf{M}^T. \quad (13)$$

Hence with Eqn. (5) and (9) one has:

$$\begin{aligned} \mathbf{S}_t &= -\mathbf{M} \sigma_0 \gamma_0^2 \mathbf{M}^T \gamma_0 \\ &= \mathbf{M} \mathbf{S}_0 \mathbf{M}^{-1}. \end{aligned} \quad (14)$$

That is - the transformation of \mathbf{S} is a similarity-transformation with a symplectic transformation matrix. The reverse transformation obviously is

$$\mathbf{S}_0 = \mathbf{M}^{-1} \mathbf{S}_t \mathbf{M}. \quad (15)$$

Now we refer to the structural identity of the matrix \mathbf{S} with the force matrix \mathbf{F} . Both are simplices and since a transformation that decouples \mathbf{F} has been shown to diagonalize the matrix \mathbf{A} of the Hamiltonian^{3,4}, it is clear that the same method can be used to diagonalize σ . The reverse of this transformation then generates the desired distribution from an initially uncorrelated σ .

Instead of a Cholesky-decomposition we may therefore use a symplectic similarity-transformation to generate the correlated distribution from an initially uncorrelated distribution. In the context of charged particle optics, the algorithm delivers even more useful information: the transformation matrix \mathbf{M}^{-1} is the transport matrix that is required to generate an uncorrelated beam.

III. SYMPLECTIC TRANSFORMATIONS AND THE ALGORITHM

The general form of a symplectic transformation matrix \mathbf{R}_b is that of a matrix exponential of a simplex γ_b multiplied by a parameter ε representing either the angle or the “rapidity”:

$$\begin{aligned} \mathbf{R}_b(\varepsilon) &= \exp(\gamma_b \frac{\varepsilon}{2}) = \mathbf{1} c + \gamma_b s \\ \mathbf{R}_b^{-1}(\varepsilon) &= \exp(-\gamma_b \frac{\varepsilon}{2}) = \mathbf{1} c - \gamma_b s, \end{aligned} \quad (16)$$

where

$$\begin{aligned} c &= \begin{cases} \cos(\varepsilon/2) & \text{for } \gamma_b^2 = -\mathbf{1} \\ \cosh(\varepsilon/2) & \text{for } \gamma_b^2 = \mathbf{1} \end{cases} \\ s &= \begin{cases} \sin(\varepsilon/2) & \text{for } \gamma_b^2 = -\mathbf{1} \\ \sinh(\varepsilon/2) & \text{for } \gamma_b^2 = \mathbf{1} \end{cases} \end{aligned} \quad (17)$$

Transformations with $\gamma_b^2 = -\mathbf{1}$ are orthogonal transformations, i.e. *rotations*, while those with $\gamma_b^2 = \mathbf{1}$ are *boosts*.

The matrix \mathbf{S} then is transformed according to:

$$\mathbf{S} \rightarrow \mathbf{R} \mathbf{S} \mathbf{R}^{-1}. \quad (18)$$

The decoupling requires a sequence of transformations, so that the RDM-coefficients of \mathbf{S} have to be recomputed after each step.

Eqn. 8 may be used to compute the RDM-coefficients s_k of the matrix \mathbf{S}

$$\mathbf{S} = \sigma \gamma_0 = \sum_{i=0}^9 s_k \gamma_k. \quad (19)$$

Numerically it is faster to analyze directly the composition. For the choice of RDMs used in Ref.^{3,4} the RDM-coefficients of \mathbf{S} as a function of σ are given by:

$$\begin{aligned} s_0 &= (\sigma_{11} + \sigma_{22} + \sigma_{33} + \sigma_{44})/4 \\ s_1 &= (-\sigma_{11} + \sigma_{22} + \sigma_{33} - \sigma_{44})/4 \\ s_2 &= (\sigma_{13} - \sigma_{24})/2 \\ s_3 &= (\sigma_{12} + \sigma_{34})/2 \\ s_4 &= (\sigma_{12} - \sigma_{34})/2 \\ s_5 &= -(\sigma_{14} + \sigma_{23})/2 \\ s_6 &= (\sigma_{11} - \sigma_{22} + \sigma_{33} - \sigma_{44})/4 \\ s_7 &= (\sigma_{13} + \sigma_{24})/2 \\ s_8 &= (\sigma_{11} + \sigma_{22} - \sigma_{33} - \sigma_{44})/4 \\ s_9 &= (\sigma_{14} - \sigma_{23})/2 \end{aligned} \quad (20)$$

Now we use the following abbreviation using the notation of 3-dimensional vector algebra:

$$\begin{aligned} \mathcal{E} &= s_0 \\ \vec{P} &= (s_1, s_2, s_3)^T \\ \vec{E} &= (s_4, s_5, s_6)^T \\ \vec{B} &= (s_7, s_8, s_9)^T, \end{aligned} \quad (21)$$

and furthermore:

$$\begin{aligned} M_r &= \vec{E} \vec{B} & \vec{r} &\equiv \mathcal{E} \vec{P} + \vec{B} \times \vec{E} \\ M_g &= \vec{B} \vec{P} & \vec{g} &\equiv \mathcal{E} \vec{E} + \vec{P} \times \vec{B} \\ M_b &= \vec{E} \vec{P} & \vec{b} &\equiv \mathcal{E} \vec{B} + \vec{E} \times \vec{P} \end{aligned} \quad (22)$$

The decoupling is done by a sequence of maximal six symplectic transformations⁴. A transformation with $\varepsilon = 0$ can be omitted. After each transformation, the RDM-coefficients s_k have to be updated and Eqns. (21) and (22) have to be re-evaluated:

1. $\mathbf{R}_0(\varepsilon)$ with $\varepsilon = \arctan(\frac{M_g}{M_r})$.
2. $\mathbf{R}_7(\varepsilon)$ with $\varepsilon = \arctan(\frac{b_x}{b_y})$.
3. $\mathbf{R}_9(\varepsilon)$ with $\varepsilon = -\arctan(\frac{b_x}{b_y})$.
4. $\mathbf{R}_2(\varepsilon)$ with $\varepsilon = \operatorname{artanh}(\frac{M_g}{b_y})$.
5. $\mathbf{R}_0(\varepsilon)$ with $\varepsilon = \frac{1}{2} \arctan(\frac{2M_b}{\vec{E}^2 - \vec{P}^2})$.
6. $\mathbf{R}_8(\varepsilon)$ with $\varepsilon = -\arctan(\frac{P_x}{P_y})$.

Given an initial covariance matrix σ_0 , the sequence of computation therefore is:

1. Compute the RDM-coefficients s_k according to Eqn. (20) and the quantities defined in Eqns. (21) and (22).
2. Compute the first (or next, resp.) transformation matrix \mathbf{R} .
3. Compute the product of the transformation matrices (and of the inverse) $\mathbf{M}_{n+1} = \mathbf{R}_{n+1} \mathbf{R}_n$.
4. Apply the first (or next, resp.) transformation $\mathbf{S}_{n+1} = \mathbf{R} \mathbf{S}_n \mathbf{R}^{-1}$.
5. Compute $\sigma_{n+1} = -\mathbf{S}_{n+1} \gamma_0$.
6. Continue with next transformation at step 1).

The six iterations yield the desired diagonal matrix σ_6 and the matrices \mathbf{M}_6 and its inverse, so that

$$\mathbf{S}_6 = \mathbf{M}_6 \mathbf{S}_0 \mathbf{M}_6^{-1}. \quad (23)$$

or:

$$\sigma_6 = \mathbf{M}_6 \sigma_0 \mathbf{M}_6^T. \quad (24)$$

The diagonal elements of σ_6 are the variances of the uncoupled gaussian distribution. Given ψ_i is the i -th uncoupled random state vector, then $\mathbf{M}_6^{-1} \psi_i$ is the corresponding state vector with the multivariate normal distribution.

IV. EXAMPLE

Consider for instance the (arbitrary) matrix of second moments σ_0

$$\begin{pmatrix} 5.8269 & -0.0303 & 0.2292 & 0.0000 & -0.0960 & 1.4897 \\ -0.0303 & 0.8851 & 0.0000 & -0.0311 & 1.8053 & -0.0015 \\ 0.2292 & 0.0000 & 3.6058 & -0.0235 & 0.0000 & 0.0000 \\ 0.0000 & -0.0311 & -0.0235 & 0.6844 & 0.0000 & 0.0000 \\ -0.0960 & 1.8053 & 0.0000 & 0.0000 & 7.0607 & -0.0224 \\ 1.4897 & -0.0015 & 0.0000 & 0.0000 & -0.0224 & 0.7304 \end{pmatrix} \quad (25)$$

The diagonal matrix σ_6 is computed to be

$$\begin{pmatrix} 1.9982 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.2984 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.1116 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.2124 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.4029 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.6637 \end{pmatrix} \quad (26)$$

Now 10^5 random vectors have been generated with a Gaussian random number generator of unit variance. The vector elements have been scaled with corresponding variances, given by the root of the diagonal elements of σ_6 and then been multiplied (or transformed) with \mathbf{M}^{-1} given by

$$\begin{pmatrix} -0.1727 & -0.0330 & 0.0081 & -1.6049 & -0.0725 & 0.1893 \\ -0.0371 & 0.3392 & 0.7051 & 0.0093 & 0.3402 & 0.1034 \\ 0.9474 & 0.1485 & 0.0008 & -0.0613 & -0.3429 & 0.9838 \\ -0.0573 & 0.5025 & -0.0072 & 0.0001 & -0.4733 & -0.1464 \\ -0.1641 & 1.6387 & 0.3732 & 0.0202 & 1.4755 & 0.4320 \\ -0.3455 & -0.0555 & 0.0042 & -0.3515 & -0.1204 & 0.3416 \end{pmatrix} \quad (27)$$

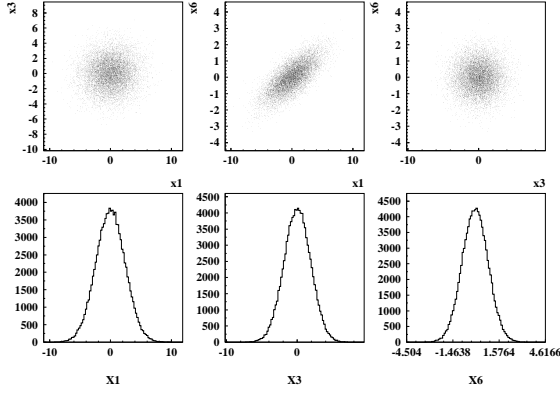


FIG. 1. Top: Correlations between several variables of the multivariate normal distribution. Bottom: The resulting probability distributions for the individual variables are again gaussian.

Then the covariance matrix of the produced random vectors was evaluated. The result is:

$$\begin{pmatrix} 5.7946 & -0.0247 & 0.2343 & -0.0060 & -0.1036 & 1.4825 \\ -0.0247 & 0.8917 & 0.0023 & -0.0306 & 1.8200 & 0.0034 \\ 0.2343 & 0.0023 & 3.5910 & -0.0299 & -0.0158 & 0.0033 \\ -0.0060 & -0.0306 & -0.0299 & 0.6849 & -0.0000 & -0.0012 \\ -0.1036 & 1.8200 & -0.0158 & -0.0000 & 7.0928 & -0.0148 \\ 1.4825 & 0.0034 & 0.0033 & -0.0012 & -0.0148 & 0.7294 \end{pmatrix} \quad (28)$$

Fig. 1 shows some of the distributions as examples.

The same procedure can be done with any initial probability distribution and the algorithm will produce the desired second moments. But the functional form of the resulting distributions of the transformed variables will only be similar to the initial distribution in the Gaussian case. Fig. 2 shows the results for the same covariance matrix if the decoupled variables have a uniform probability distribution, but same variances. The covariance matrix is correctly reproduced.

V. CONCLUSION

The method of symplectic decoupling of linearly coupled variables has been applied to the problem of multivariate random distributions. It has been shown that the use of symplectic algebra has severe advantages: The same methods can be applied to solve a variety of problems. The presented algorithm is especially interesting for the generation of starting conditions of particle tracking codes like - for example - OPAL^{1,2}.

In cases where the decoupled process is known to have a non-Gaussian probability distribution and if the transport matrix \mathbf{M} of a linear transport system is known, it should be possible to derive unknown parameters of the initial distribution by comparison with the computed expected distribution. Fig. 2 shows that a flat distribution yields a clear “signature”.

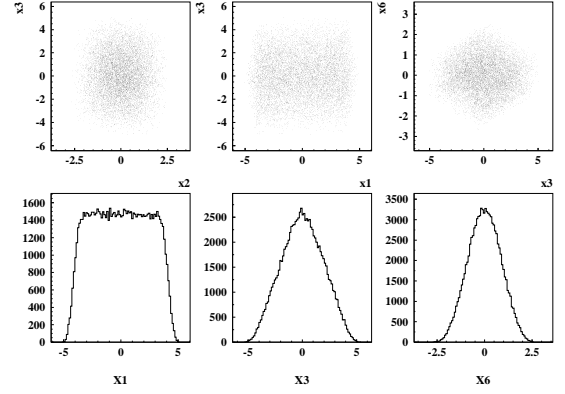


FIG. 2. Top: Correlations between several variables of the multivariate flat distribution. Bottom: The resulting probability distributions for the individual variables strongly depend on the correlations. The stronger the correlations, the more gaussian the distribution will be (central limiting theorem).

ACKNOWLEDGMENTS

The software used for the computation has been written in “C” and been compiled with the GNU[©]-C++ compiler 3.4.6 on Scientific Linux. The CERN library (PAW) was used to generate the figures.

Appendix A: The γ -Matrices

The real Dirac matrices used throughout this paper are:

$$\begin{aligned} \gamma_0 &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} & \gamma_1 &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \\ \gamma_2 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} & \gamma_3 &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix} \\ \gamma_{14} &= \gamma_0 \gamma_1 \gamma_2 \gamma_3; & \gamma_{15} &= \mathbf{1} \\ \gamma_4 &= \gamma_0 \gamma_1; & \gamma_7 &= \gamma_{14} \gamma_0 \gamma_1 = \gamma_2 \gamma_3 \\ \gamma_5 &= \gamma_0 \gamma_2; & \gamma_8 &= \gamma_{14} \gamma_0 \gamma_2 = \gamma_3 \gamma_1 \\ \gamma_6 &= \gamma_0 \gamma_3; & \gamma_9 &= \gamma_{14} \gamma_0 \gamma_3 = \gamma_1 \gamma_2 \\ \gamma_{10} &= \gamma_{14} \gamma_0 = \gamma_1 \gamma_2 \gamma_3 & \gamma_{11} &= \gamma_{14} \gamma_1 = \gamma_0 \gamma_2 \gamma_3 \\ \gamma_{12} &= \gamma_{14} \gamma_2 = \gamma_0 \gamma_3 \gamma_1 & \gamma_{13} &= \gamma_{14} \gamma_3 = \gamma_0 \gamma_1 \gamma_2 \end{aligned} \quad (A1)$$

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